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A Full 2-D Parallel Implementation of CH3D-Z

by

Clint Dawson
Victor Parr

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Clint Dawson and Victor Parr
The University of Texas at Austin

1 Introduction

CH3D-Z is a well-known hydrodynamic, salinity and temperature model developed at the U.S. Army Engineer Research and Develpment Center (ERDC), in Vicksburg, MS [1]. In CH3D-Z, finite differences are used to replace derivatives in the governing equations, resulting in a system of linear algebraic equations. The code solves external mode equations for depth-averaged velocities and surface elevations, and internal mode equations to account for three-dimensional variations in velocities, temperature and salinity.

The external mode consists of a continuity equation for the water surface elevation ζ and vertically integrated momentum equations for the depth-averaged horizontal velocities $\overline{U}$ and $\overline{V}$. The external mode equations in computational space are given by:

$$\frac{\partial \zeta}{\partial t} + \beta\left(\frac{\partial \overline{U}}{\partial \xi} + \frac{\partial \overline{V}}{\partial \eta}\right) = 0, \quad (1)$$

$$\frac{\partial \overline{U}}{\partial t} + \frac{H}{J^2} G_{22} \frac{\partial \zeta}{\partial \xi} = M, \quad (2)$$

$$\frac{\partial \overline{V}}{\partial t} + \frac{H}{J^2} G_{11} \frac{\partial \zeta}{\partial \eta} = N, \quad (3)$$

where ζ and η are the computational variables, J is the Jacobian of the transformation from physical to computational space, and where M and N include advective and forcing terms.

CH3D-Z approximates (1)-(3) using finite differences, based on a staggered grid approach, where elevations are approximated at the cell centers, and velocities are approximated at the cell edges. Let i, j subscripts denote the value of ζ at the center of grid block i, j, the value of $\overline{U}$ on the left edge of the grid block, and the value of $\overline{V}$ on the bottom edge of the grid block.

In the original solver the values at the new time step were computed by using the following equations in a ξ-sweep and an η-sweep.

The ξ - sweep :

$$
\begin{aligned}
\zeta^{*}_{ij} + \frac{\beta\theta\Delta t}{\Delta\xi}(\overline{U}^{*}_{i+1,j} - \overline{U}^{*}_{i,j}) &= \zeta^{n}_{i,j} \\
&\quad -(1-\theta)\frac{\Delta t}{\Delta\xi}(\overline{U}^{n}_{i+1,j} - \overline{U}^{n}_{i,j}) \\
&\quad -\frac{\Delta t}{\Delta\eta}(\overline{V}^{n}_{i,j+1} - \overline{V}^{n}_{i,j}).
\end{aligned} \tag{4}
$$

$$
\begin{aligned}
\overline{U}^{n+1}_{i,j} + \frac{\theta\Delta t H G_{22}}{\Delta\xi J^2}(\zeta^{*}_{i,j} - \zeta^{*}_{i-1,j}) &= \overline{U}^{n}_{i,j} \\
&\quad -(1-\theta)\frac{\theta\Delta t H G_{22}}{\Delta\xi J^2}(\zeta^{n}_{i,j} - \zeta^{n}_{i-1,j}) \\
&\quad +\Delta t M^n.
\end{aligned} \tag{5}
$$

The η - sweep :

$$
\begin{aligned}
\zeta^{n+1}_{ij} + \frac{\beta\theta\Delta t}{\Delta\eta}(\overline{V}^{n+1}_{i,j+1} - \overline{V}^{n+1}_{i,j}) &= \zeta^{*}_{i,j} \\
&\quad -(1-\theta)\frac{\Delta t}{\Delta\eta}(\overline{V}^{n}_{i,j+1} - \overline{V}^{n}_{i,j}) \\
&\quad -\frac{\Delta t}{\Delta\eta}(\overline{V}^{n}_{i,j+1} - \overline{V}^{n}_{i,j}).
\end{aligned} \tag{6}
$$

$$
\begin{aligned}
\overline{V}^{n+1}_{i,j} + \frac{\theta\Delta t H G_{11}}{\Delta\eta J^2}(\zeta^{n+1}_{i,j} - \zeta^{n+1}_{i,j-1}) &= \overline{V}^{n}_{i,j} \\
&\quad -(1-\theta)\frac{\theta\Delta t H G_{11}}{\Delta\eta J^2}(\zeta^{n}_{i,j+1} - \zeta^{n}_{i,j}) \\
&\quad +\Delta t N^n.
\end{aligned} \tag{7}
$$

Here we have suppressed the spatial dependence of the coefficients G_{11}, G_{22} and J, which involve the mapping from the physical domain to the computational grid.

This alternating direction type approach inhibits parallelization, at least in a domain decomposition sense. We modified the time discretization in CH3D-Z by modifying the continuity equation (4) to be implicit in ζ, $\overline{U}$ and $\overline{V}$. Also, (5) is implicit in $\overline{U}$ and ζ and (7) is implicit in $\overline{V}$ and ζ. Substituting into the continuity equation we obtain the single equation in ζ:

$$\begin{aligned}
2[1 + (\frac{\beta\theta\Delta t}{\Delta\xi})(\frac{\theta\Delta t H G_{22}}{\Delta\xi J^2}) + & \\
(\frac{\beta\theta\Delta t}{\Delta\eta})(\frac{\theta\Delta t H G_{11}}{\Delta\eta J^2})]\zeta_{i,j}^{n+1} & \\
-[(\frac{\beta\theta\Delta t}{\Delta\xi})(\frac{\theta\Delta t H G_{22}}{\Delta\xi J^2})]\zeta_{i-1,j}^{n+1} & \\
-[(\frac{\beta\theta\Delta t}{\Delta\xi})(\frac{\theta\Delta t H G_{22}}{\Delta\xi J^2})]\zeta_{i+1,j}^{n+1} & \\
-[(\frac{\beta\theta\Delta t}{\Delta\eta})(\frac{\theta\Delta t H G_{11}}{\Delta\eta J^2})]\zeta_{i,j-1}^{n+1} & \\
-[(\frac{\beta\theta\Delta t}{\Delta\eta})(\frac{\theta\Delta t H G_{11}}{\Delta\eta J^2})]\zeta_{i,j+1}^{n+1} & = R1_{i,j} \\
& -\frac{\beta\theta\Delta t}{\Delta\xi} R2_{i+1,j} + \frac{\beta\theta\Delta t}{\Delta\xi} R2_{i,j} \\
& -\frac{\beta\theta\Delta t}{\Delta\eta} R3_{i,j+1} + \frac{\beta\theta\Delta t}{\Delta\eta} R3_{i,j} \qquad (8)
\end{aligned}$$

where :

$$\begin{aligned}
R1_{i,j} &= \zeta_{i,j}^n - (1-\theta)\frac{\Delta t}{\Delta\xi}(\overline{U}_{i+1,j}^n - \overline{U}_{i,j}^n) - \frac{\Delta t}{\Delta\eta}(\overline{V}_{i,j+1}^n - \overline{V}_{i,j}^n) \\
&\quad + \zeta_{i,j}^n - (1-\theta)\frac{\Delta t}{\Delta\eta}(\overline{V}_{i,j+1}^n - \overline{V}_{i,j}^n) + \frac{\Delta t}{\Delta\eta}(\overline{V}_{i,j+1}^n - \overline{V}_{i,j}^n) \\
R2_{i,j} &= \overline{U}_{i,j}^n - (1-\theta)\frac{\Delta t H G_{22}}{\Delta\xi J^2}(\zeta_{i,j}^n - \zeta_{i-1,j}^n) + \Delta t M^n \\
R3_{i,j} &= \overline{V}_{i,j}^n - (1-\theta)\frac{\Delta t H G_{11}}{\Delta\eta J^2}(\zeta_{i,j+1}^n - \zeta_{i,j}^n) + \Delta t N^n
\end{aligned}$$

Using this equation we can assemble a matrix which is then solved using the NSPCG package to yield ζ at the new time step. $\overline{U}$ and $\overline{V}$ at the new time step are then retrieved using the modified equations (5) and (7).

Once ζ, $\overline{U}$ and $\overline{V}$ have been calculated, the code then computes three-dimensional velocities u, v and w through a so-called "internal mode" computation, which involve solving tridiagonal systems over the vertical water column. Finally, salinity and temperature are updated, appropriate output variables are written to disk, and the code proceeds to the next time step.

During the first part of this project year, we slightly modified the system above by multiplying (8) by $G_{22}G_{11}$. The effect of this modification is to make the system in ζ symmetric, positive definite. Thus, preconditioned conjugate gradient techniques can easily be applied to this system.

2 Parallelization Details

The approach we are taking to parallelizing the code is very similar to the strategy we have used in previous parallelizations of CE-QUAL-ICM and ADCIRC. This approach involves

- Development of a preprocessor, which divides the computational domain into subdomains, one for each processor, then partitions the data into subdomain data, to be read by each processor. We have used the METIS package for performing the partitioning, because it gives reasonably shaped subdomains with load balancing across processors.

- Message passing calls are then added to the code, to pass information from one subdomain to another. The primary message passing is in the linear solution step described above. In particular, at each linear iteration, elevation unknowns and global sums (inner products) must be passed among the processors. There are several other places in the code where message passing must also be performed, for example, at the end of the salinity and temperature calculations.

- Development of a postprocessor, which takes the output from each subdomain and merges it into a global output file.

As of now, we have essentially completed steps 1 and 2, and are in the process of testing the parallel code for a data set of Chesapeake and Delaware Bays, and the CND Canal. The preprocessor has been developed and debugged. A decomposition of the computational domain into two subdomains

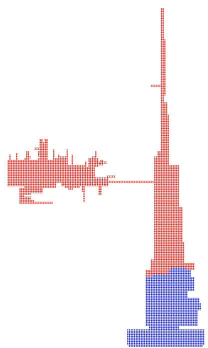

Figure 1: Two subdomain decomposition of the Chesapeake-Delaware-CND Canal domain

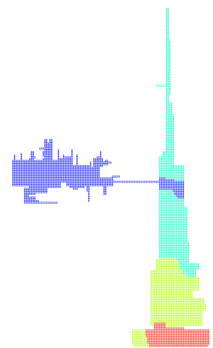

Figure 2: Four subdomain decomposition of the Chesapeake-Delaware-CND Canal domain

is given in Figure 1, and a four subdomain decomposition is given in Figure 2. Again, these decompositions are performed using the METIS software package.

Message passing calls have been added to appropriate locations in the original CH3D-Z code. Part of the difficulty in our parallelization effort has been the **amount of hardwired code** we have had to deal with, specific to this case. There are numerous sections in the code where specific array locations are modified based on some physical condition (e.g. boundary condition, channel, etc.).

3 Test runs

The parallel code has been tested on the Chesapeake Bay data set provided by ERDC. The simulated time in this run is 1 day, or 960 time steps. In this run, the domain is divided into two subdomains. Surface elevations for the parallel code and the serial code have been compared, and we see agreement between the two solutions to eight significant digits. Therefore, the parallel code seems to be producing correct results. The elevation solution after 960 time steps is shown in Figure 3.

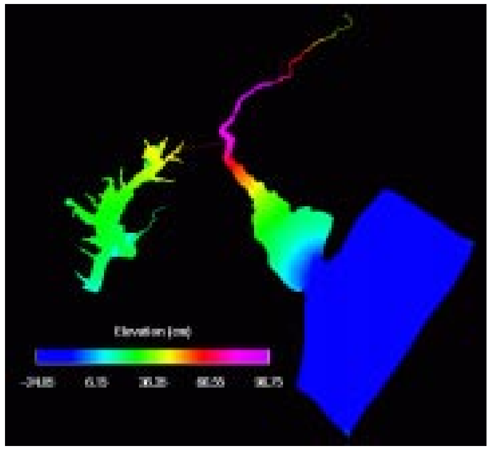

Figure 3: Surface elevation for the Chesapeake-Delaware-CND Canal problem after 1 day.

4 Conclusions

A full two-dimensional parallel implementation of CH3D-Z has been undertaken. Testing of the parallel version is still underway, but preliminary results indicate that the parallel code produces correct results, at least for a decomposition into two subdomains. Further testing for more subdomains, and parallel scaling studies will be performed in the near future.

References

[1] B.H. Johnson, R.E. Heath, B.B. Hsieh, K.W. Kim and H.L. Butler, *Development and verification of a three-dimensional numerical hydrodynamic, salinity, and temperature model of Chesapeake Bay, Volume 1*, Technical Report HL-91-7, Department of the Army, Waterways Experiment Station, Corps of Engineers, 3909 Halls Ferry Road, Vicksburg, MS, 39180-6199, 1991.